Surrogate-based Evolutionary Optimization Using Computationally Expensive Simulations

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Overview

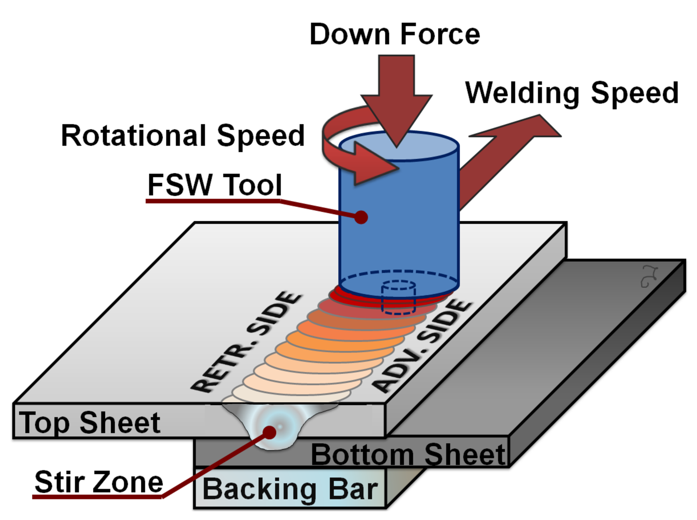
Optimizing physical processes and functions is key to problem solving in many practical fields. Classical techniques such as genetic algorithms and gradient descent require thousands of evaluations which is often not practically possible due to limited resources and time. Computer simulations capable of replicating the results of some complex process can be used to save resources, but they still suffer from time costs. The goal of surrogate assisted optimization is to find the optimal solution with few expensive evaluations.

In this work we:

- Introduce a novel constraint-handling methodology grounded in the surrogate-based optimization framework
- Show that our methodology achieves superior results in less time than state-of-the-art
- Apply the proposed method to Friction Stir Welding and other problems

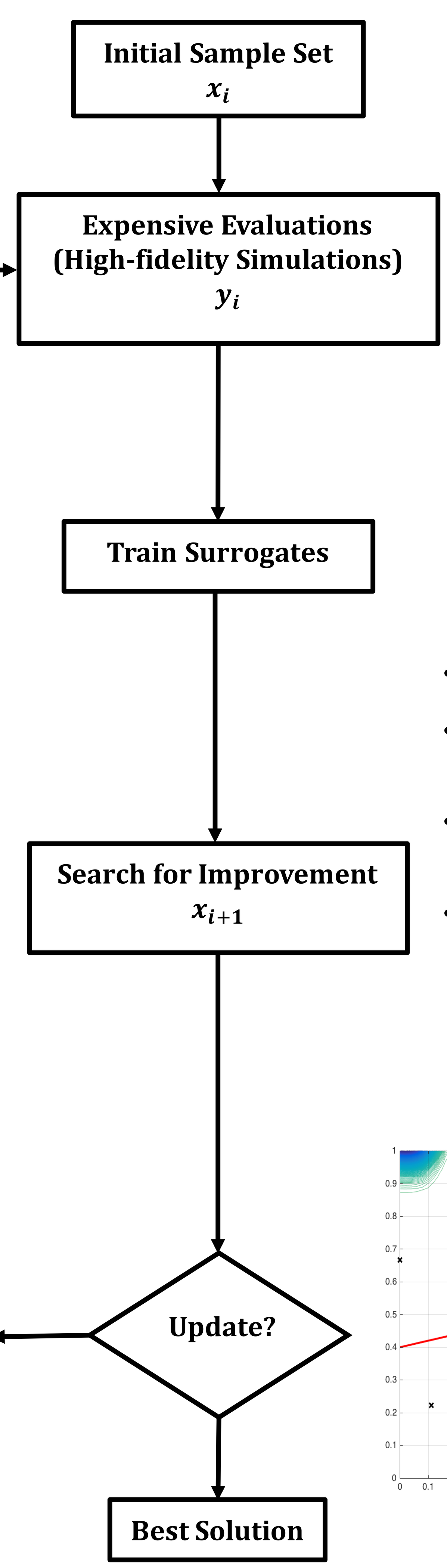
Friction Stir Welding

- Widespread use in aerospace and automotive industries to join two pieces of metal with frictional heating and plastic deformation as a result of heated stirring action
- **Four design variables** – radius of tool shoulder, radius of probe, welding speed, and tool rotational speed
- **Three constraints** – two constraints restrict the average temperature of the shoulder layer on both sides, third constraint ensures the temperature of material in front of probe is high enough



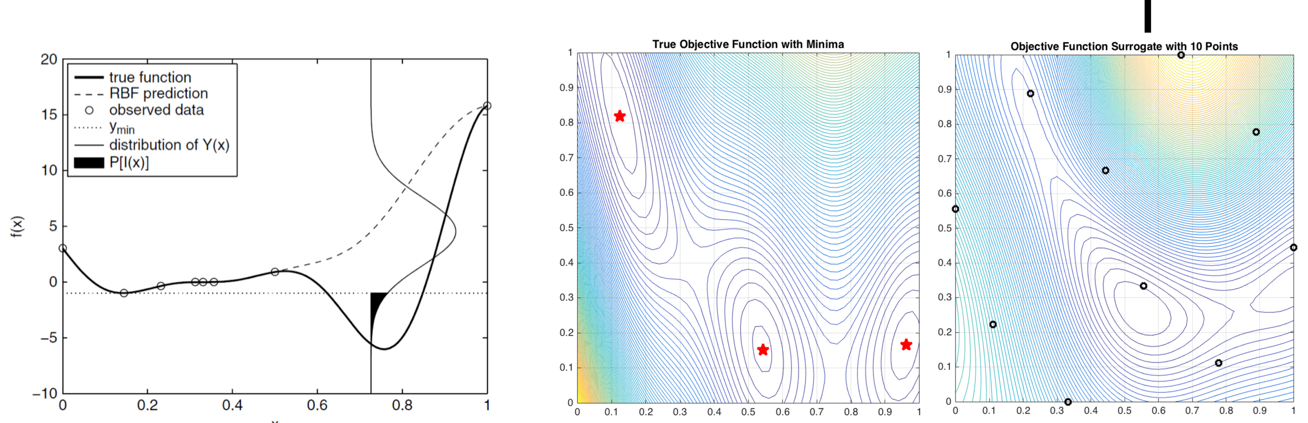
Surrogate Assisted Optimization with Constraint Handling

Surrogate Assisted Optimization

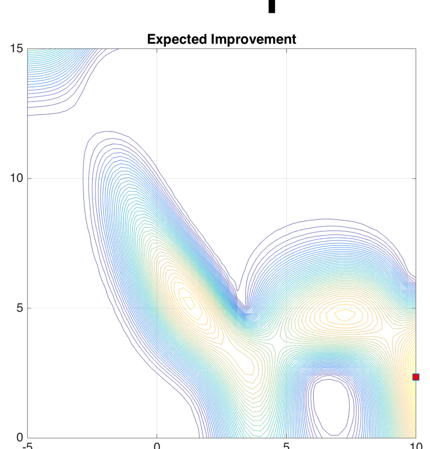


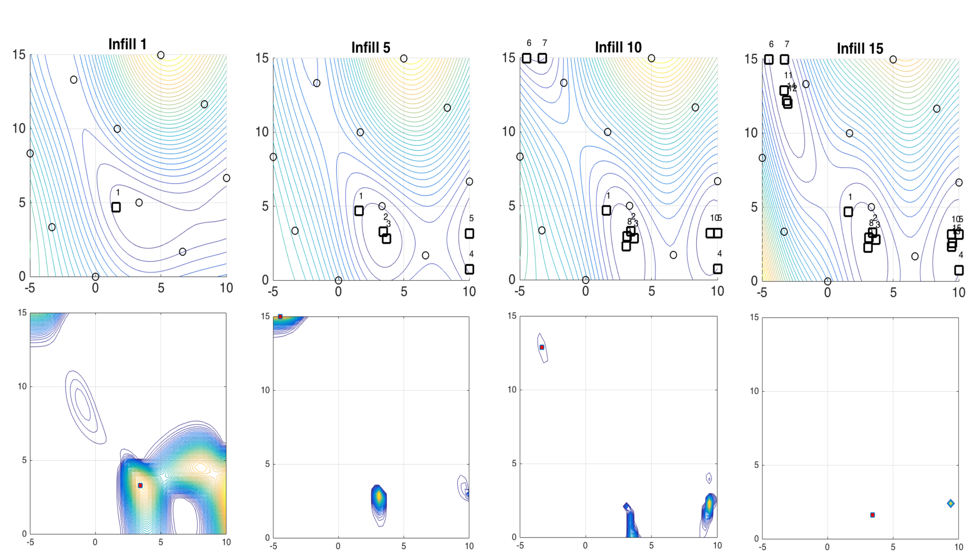
Optimization

- Initial dataset has known points evaluated using the expensive function, $\mathcal{D} = \{(x_i,\ y_i) \mid i = 1, \ldots, n\}$
- Build a Gaussian Process model with squared-exponential covariance function. Hyperparameters found by maximizing likelihood capture underlying patterns among observed points
- Compute $p(y|x_*, \mathcal{D})$ for y values at candidate locations x_*. The mean is our best prediction for that point and the variance represents the uncertainty in our prediction.



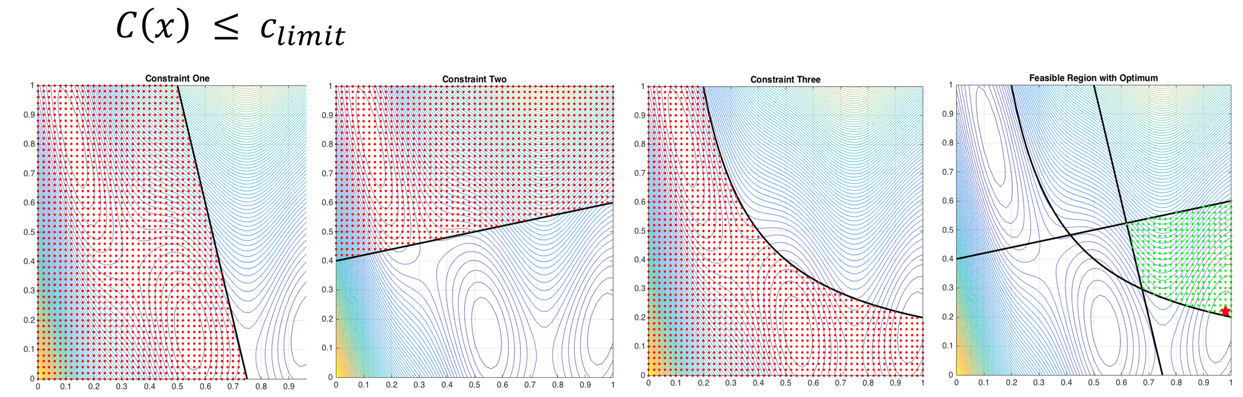
- Given predictions for unknown points, maximize the *expected improvement* (EI) criterion, $E[I(x)]$
- Chosen point makes a trade-off between exploitation and exploration by utilizing uncertainty in predictions
- Evaluate the expensive function at this location and update the model





Constraint Handling

- Real world optimization problems almost always include a set of constraints that model inherent physical limitations.
- Deem a portion of the input space as infeasible and must be incorporated into the general optimization framework to avoid invalid solutions
- A solution is infeasible if it violates one or more constraints $C(x) \leq c_{limit}$

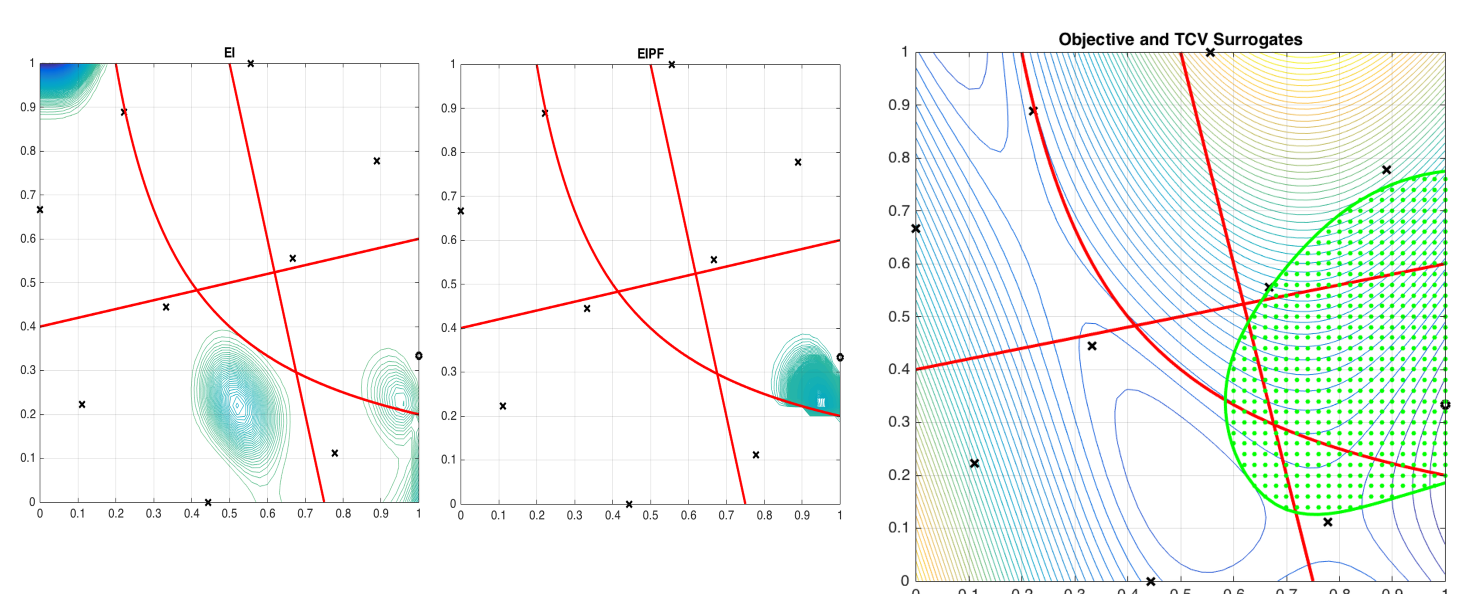


EIPF

- Surrogate for each constraint
- $E[I(x) \cap F(x)] = E[I(x)] \times P[F_1(x)] \times P[F_2(x)] \times P[F_3(x)]$
- Computationally expensive and scales poorly
- EIPF values vanish for problems with many constraints

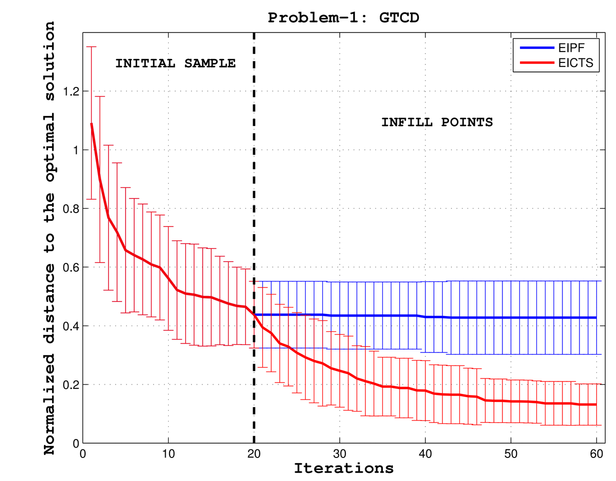
EICTS

- One surrogate that captures all constraint information, *Total Constraint Violation* (TCV)
- TCV – If infeasible, only sum violations (positive). If feasible, sum all constraint outputs (negative)
- Maximize EI using *Constrained Tournament Selection* – genetic algorithm with modified selection operator
- CTS – favor individuals with negative TCV and high EI values

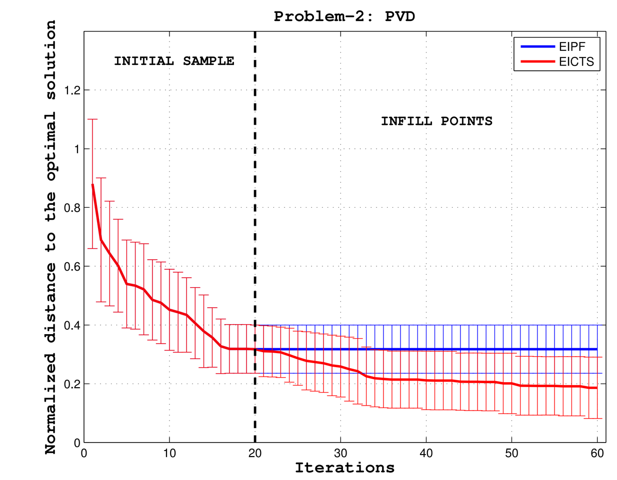


Results

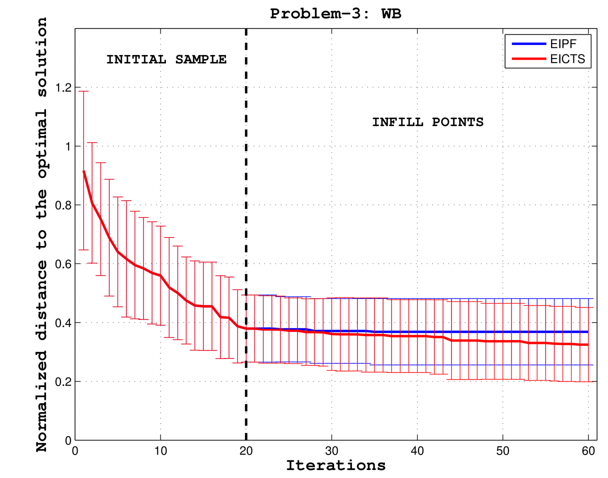
EICTS is compared with EIPF on three validation problems. Problem 4 shows the results of optimizing the Fraction Stir Welding process.



Gas Transmission Compressor Design
4 variables, 1 constraint



Pressure Vessel Design
4 variables, 3 constraints



Welded Beam
4 variables, 6 constraints

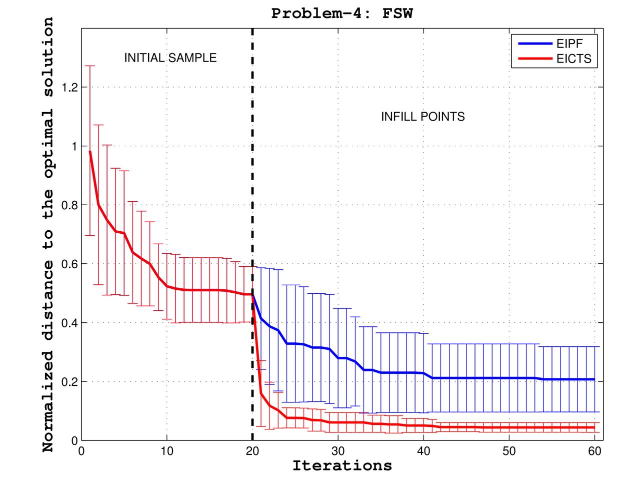


Table compares averages across 30 trials each with 40 iterations:

1) number of feasible solutions
2) Runtime in seconds
3) Fitness of best solution

Performance Criterion	Problem	EIPF	EICTS
$n_{feas,avg}$	GTCD	41.467	20.300
	PVD	0.3667	1.2667
	WB	None	0.0333
	FSW	15.500	6.7500
$CPU - time_{avg}$	GTCD	225.95	214.63
	PVD	353.15	210.53
	WB	702.25	213.56
	FSW	5385.3	3797.8
$Fitness_{feas,best}$	GTCD	4,075,744.10	3,035,175.86
	PVD	6680.9	6049.2
	WB	None	5.195
	FSW	3.722	3.693

Conclusion and Future Work

- A new efficient constraint handling methodology was developed and applied to a real world design problem. **This work is accepted at IEEE World Congress on Computational Intelligence.**
- EICTS finds better solutions with a ~1.5x increase in runtime performance
- EICTS uses two surrogates total for any given problem, one for the objective function and one for the *Total Constraint Violation*
- TCV scales to the entire number line, assigning positive values for feasible solutions and negative values for infeasible solutions, allowing for smoother prediction models. Use of *Constrained Tournament Selection* ensures there is no favorability in the magnitude of feasibility.
- Future work involves expanding the range of practical problems solved using EICTS and extending the method for multi-objective optimization.
- Examples of interesting problems include optimizing the structure of a cardiovascular stent in Balloon Angioplasty, locating WiFi devices using sparse RSSI signals